Analysis of water transport in unsaturated conditions comparison between labcrete and fieldcrete

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2 comparison between labcrete and fieldcrete

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8 **Abstract**

9 The differences in unsaturated permeability between concrete prepared in the laboratory

10 (labcrete) and on a real construction site (fieldcrete) were investigated experimentally and

11 using inverse analysis. Although more porous, the fieldcrete specimens were shown to have an

12 average permeability very close to the labcrete ones. The fieldcrete permeabilities also exhibited

13 more variability than the labcrete ones. Numerical simulations performed on 3D reconstructed

14 concrete specimens showed that differences in coarse aggregate distribution cannot explain the

15 variability observed at the macroscopic scale and that an important part may originate from the

16 properties of mortar matrix.

17 **Keywords:** labcrete; fieldcrete; permeability; inverse analysis; 3D mesostructure.

18 1. Introduction

19 The amount of evaporable water that is present in the porosity of concrete is of paramount

20 importance for the durability of reinforced concrete structures: (1) because it influences the

21 concrete transport properties and then the ingress rate of aggressive species such as CO_2 or

22 chlorides [1–5]; (2) because the poral solution is the medium that allows chemical reactions to

23   occur such as carbonation or rebar corrosion [6–8] and also (3) because the loss of water

24   induces shrinkage and possibly cracking [9–11] Describing water exchange between a concrete

25   structure and the surrounding environment is then the first and inevitable step towards

26   durability assessment.

27   Among the data needed to describe water transport, the permeability is of first importance: it

28   accounts for the ability of a fluid (water in our case) to pass through concrete due to pressure

29   gradient. Permeability is considered as a relevant durability index for service-life prediction

30   [12–16] and is measured to verify whether the concrete composition complies with the

31   specifications. To this end, characterization tests are generally performed using specimens

32   prepared in the laboratory ('labcrete'). This approach may be regarded as inconsistent because

33   it does not account for the properties of the concrete that is prepared and used onsite

34   ('fieldcrete') [17,18]. Labcrete specimens are generally prepared with great care by experienced

35   technicians and/or scientists using batches of small volume, in controlled environmental

36   conditions and are carefully vibrated and cured whereas fieldcrete is generally prepared in

37   much larger batches in concrete plants in uncontrolled environmental conditions before further

38   use by onsite workers [18,19]. Fieldcretes are then likely to be of lower quality than labcretes in

39   terms of mechanical as well as durability properties; the question is how much?

40   There are very few studies in the literature that compare the properties of labcrete and

41   fieldcrete. However, fieldcretes are known to exhibit reduced compressive strength compared to

42   labcretes and the difference is about 10-15% [20,21]. Unexpectedly, no significant differences in

43   chloride diffusion coefficient between laboratory and field measurements were obtained over a

44   large panel of concretes by [22,23], indicating that fieldcretes and labcretes would be similar in

45   terms of diffusion properties. The available results about permeability tell a different story.

46   Using gas, the permeability of fieldcrete was shown to be greater than that of the labcrete up to

47   four times [24–26]. The same applies to the studies of Diaz *et al*. [27] who used the Torrent

48   permeameter to measure the permeability of low-carbon concrete elements exposed to marine

49   environment *in situ* as well as companion specimens in the laboratory. The field measurements

50   were up to 8 times higher than the laboratory ones. This discrepancy may be due to differences

51   in properties of lab- and fieldcrete but also to differences in water content between the

52   laboratory and field specimens [28] and to the absence of proper cure for the fieldcrete [29,30].

53   The objective of this study is to investigate the differences in water permeability in unsaturated

54   conditions between a labcrete (concrete prepared and cured in the laboratory) and the

55   corresponding fieldcrete (same formulation of concrete prepared on a construction site); this is

56   obviously lacking in the scientific literature. The influence of the on-site cure (*e.g.* early-age

57   drying) and structural effects (*e.g.* cracking) is not addressed in this article and should be the

58   subject of a further study. Specifically, mass loss due to drying of several specimens from

59   saturation up to 30% of relative humidity is measured. The results are then used for identifying

60   by inverse analysis and comparing the parameters of a classical model describing the water

61   transfer via a single mass balance equation. Besides this experimental procedure, one-

62   dimensional numerical simulations are performed to analyze the sensitivity of the saturation

63   profiles towards the identified materials parameters. Further, 3D simulations on mesoscale

64   concrete specimens exhibiting different aggregate distributions are performed to investigate

65   more precisely local effects due to the presence of aggregates on the saturation degree.

2. Material and methods

2.1. Concrete

68   The concrete used in this study was designed by the Belgian agency for radioactive waste and

69   enriched fissile materials (ONDRAF-NIRAS[1]) in the framework of a project of Low-Level

70   radioactive waste surface disposal in Dessel, Belgium (Ondraf-Niras, 2010). It is a modern

71   concrete including CEM I (Ordinary Portland Cement) with a water-to-cement ratio of 0.47. The

72   superplasticizer (Masterglenium® 27) content was adjusted so that the slump of the fresh mix

73   would reach 19 cm. The average compressive strength at 28 days is equal to 49 MPa using

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[1] http://www.nirond.be

74 cylinders (68 MPa was obtained using cubes). A large experimental campaign was undertaken at

75 the Eduardo Torroja Institute (IeTcc[2]) in which many characterization tests were conducted on a

76 preliminary but very similar composition [31] along with a sensitivity analysis at the Belgian

77 Building Research Institute [32], demonstrating its robustness. Among all of them the first

78 desorption isotherm was acquired. This concrete (Table 1) was studied in laboratory and was

79 also produced in industrial conditions for the realization of test panels (11 m height, 3 m long) to

80 verify its feasibility for the construction of surface disposal modules in Dessel. Up to this day,

81 three test panels have been erected with this composition, each of them containing about 25 m^3

82 concrete. About 6 to 10 batches were furnished during the construction of each test panel. The

83 fieldcrete used in this study was produced during one of these test panels. The cubes were

84 fabricated on-site by the site workers. They were unmolded the day after casting and they were

85 then kept in a humid chamber (RH>95%, *ca*. 20°C) for 28 days. After that, the specimens were

86 kept under water at ambient temperature for multiple months before use.

87 In the laboratory the concrete (labcrete) was mixed in small batches (30 L) and cylindrical

88 specimens (Ø11×H22 cm) were prepared that were normally vibrated and then kept in their

89 sealed molds before use.

90 *Table 1 – composition of the concrete*

Compound	Nature	Quantity (kg/m^3)
Low-heat cement	CEM I 42.5 LH	360
Filler	Limestone (Calcitec)	40
Water		169
Gravel 6/20 mm	Limestone	472
Gravel 6/14 mm	Limestone	200
Gravel 2/6 mm	Limestone	417
Sand 0/4 mm	Limestone	721
Superplasticizer	Glenium 27 (BASF)	1.8 (0.5 wt% of cement)

91

[2] http://www.ietcc.csic.es/index.php/en/

2.2. Methods

Four mature labcrete specimens (Ø11×H22 cm), that were kept two years in their sealed molds after casting, were cored to generate 4 smaller cylinders (Ø6×H22 cm). Top and bottom ends, whose properties may differ from the bulk [33–36], were sawn and thrown away. This resulted in four new cylinders (Ø6×H15 cm) that assumedly exhibited uniform properties. In the same way, five mature fieldcrete cubes (15×15×15 cm), originating from five different batches, were cored to generate two smaller cylinders (Ø6×H15 cm): 2 cylinders per cube. They were cut as described above resulting in ten new cylinders (Ø6×H11 cm).

All the specimens were resaturated under water and vacuum [37] and the volume and density of each specimen were measured using the buoyancy method (Table 2). All the saturated cylinders were introduced in a climatic chamber at 25 °C and 55% RH for 230 days. The RH within the chamber was then lowered to 30% for 105 more days. At given times, the chamber was opened and the specimens' weight was measured to monitor their drying. Eventually, all the specimens were completely dried at 105 °C for porosity evaluation.

2.3. Permeability assessment (inverse analysis)

The intrinsic permeability of the concrete was evaluated using inverse analysis [38–40]. Water transport in unsaturated concrete was described making use of a simplified approach accounting for liquid water permeation only. The contribution of other motions (gas phase permeation and diffusion of vapor) was neglected [38]. Finally, the only differential equation to solve was the following [41,42]:

$$\phi \left(\frac{\partial S}{\partial P} \right) \frac{\partial P}{\partial t} = \operatorname{div} \left[\frac{K k_r}{\eta} \operatorname{grad}(P) \right] \tag{1}$$

with:

- ϕ the concrete porosity (without unit)
- S the saturation degree of the porosity (without unit)
- P the water pressure within the pores (Pa)

116   • η the water viscosity (Pa s)

117   • K the intrinsic permeability (m²)

118   • k_r the relative permeability to water (without unit)

119   The equation proposed by van Genuchten [43] was used to describe the water retention curve:

$$S = \left[1 + \left(\frac{P}{P_0}\right)^{\frac{1}{1-m}}\right]^{-m} \tag{2}$$

120   where m and P_0 are two positive parameters that were identified using the experimental

121   desorption isotherm measured at 20°C at IETcc [31]. The following resulting values were

122   obtained: $m = 0.532$ and $P_0 = 59.05$ MPa. It must be mentioned that the fieldcrete desorption

123   isotherm was not measured and that a unique dataset was considered here: *i.e.* the desorption

124   isotherm was assumed to be the same for the labcrete and for the fieldcrete. Fieldcretes are

125   known to present more variability than labcretes [44]. Using fieldcrete specimens from different

126   batches was then expected to possibly induce modifications in their desorption isotherm

127   [44,45]. It should also be quoted that using different isotherm data for the labcrete and the

128   fieldcrete might have yielded (slightly) different results in permeability [42]; however,

129   considering variable isotherm curves was deemed unreasonable due to the number of tests that

130   should have been conducted to characterize the desorption isotherm of all the specimens and

131   the considerable time that would have been required.

132   Following the proposition of Savage and Janssen [46], Mualem's model [43,47] was used to

133   assess the relative permeability to water k_r:

$$k_r = \left[1 + \left(\frac{P}{P_0}\right)^{\frac{1}{1-m}}\right]^{-m\alpha} \left\{1 - \left(\frac{P}{P_0}\right)^{-\frac{m}{1-m}}\left[1 + \left(\frac{P}{P_0}\right)^{\frac{1}{1-m}}\right]^{-m}\right\}^2 \tag{3}$$

134   where α is the pore-interaction factor. It is a lumped parameter that accounts for the

135   connectivity and tortuosity of the pore network. Mualem [47] suggested to use $\alpha = +0.5$ as

136   default value and so it has been extensively used so far. It was however shown that using

137     $\alpha = +0.5$ could sometimes result in inacceptable fits [48] and that α could exhibit very different

138   values either positive or negative [49,50].

139   The left-hand term of eq. *(1)* was easily obtained by derivation of eq. *(2)*:

$$\phi\left(\frac{\partial S}{\partial P}\right) = -\frac{m\phi}{(m-1)P_0}\left(\frac{P}{P_0}\right)^{\frac{m}{1-m}}\left[1 + \left(\frac{P}{P_0}\right)^{\frac{1}{1-m}}\right]^{-1-m} \tag{4}$$

140   In practice, eq. (1) was solved using the finite-element method and the code Cast3m[3]. In

141   accordance with the symmetry of the problem, the mesh only accounted for a sample quarter in

142   axisymmetric conditions (Figure 1): 75×150 four-node quadrangles were used in a non-uniform

143   grid. The initial conditions were uniform temperature T_0 = 298.15 K (25 °C) and water pressure

144   P_0 = 0.0 MPa (the samples were initially saturated). The boundary conditions were (for time $t \geq$

145   0): T = 298.15 K and P = -82.1 MPa for the 230 first days (55% RH) and then P = -165.3 MPa for

146   the rest of the simulation (30% RH). Please note that Kelvin's equation *(5)* was used to calculate

147   the water pressure P generated by the relative humidity h:

$$P = \rho\frac{RT_0}{M}ln(h) \tag{5}$$

148   with:

149   • R the universal gas constant (8.3145 J/mol/K)

150   • ρ and M the water density (997.1 kg/m³) and molar mass (0.018 kg/mol) respectively
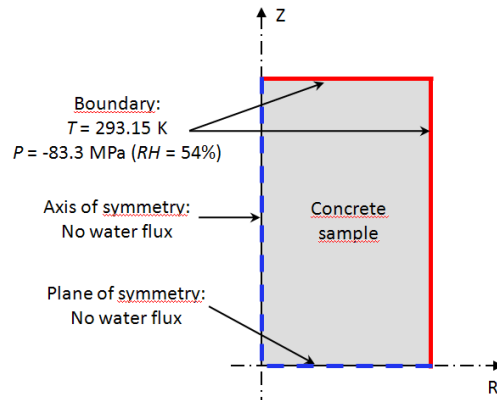
151   The intrinsic permeability K was then evaluated through the minimization of the quadratic

152   difference between the computed and measured mass variations:

$$F = \sum_{j=1}^{N}\left[\left(\frac{\Delta m}{m}\right)_j^{exp} - \left(\frac{\Delta m}{m}\right)_j^{sim}\right]^2 \tag{6}$$

153   with:

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[3] http://www-cast3m.cea.fr/

158

159 *Figure 1 – schematic description of the mesh and boundary conditions*

3. Results

160

3.1. Density and porosity

161

162 Table 2 presents the density and porosity results. It is interesting to note that the porosity of the

163 fieldcrete (11.9%) was greater than that of the labcrete (10.6%). This was consistent with the

164 density results: the density of the fieldcrete (2.432) was found to be lower than that of the

165 labcrete (2.472). Moreover the intrinsic permeability of the fieldcrete was always greater than

166 that of the labcrete, irrespective of the RH-step, and the experimental scatter obtained for the

167 fieldcrete is about seven times greater than that of the labcrete. This was believed to be due to

168 the increased difficulty of the concreting operations on site as well as to the five different

169 batches [44].

170

171

Table 2 – density and porosity of the concrete specimens

Concrete	Batch	Specimen	Density		Porosity	
			Individual value	Average (COV)	Individual value	Average (COV)
Labcrete	1	I	2.474	2.472 (0.1%)	10.6%	10.6% (0.8%)
		II	2.469		10.7%	
		III	2.471		10.7%	
		IV	2.472		10.6%	
Fieldcrete	1	1-1	2.421	2.432 (0.6%)	12.1%	11.9% (6.5%)
		1-2	2.455		11.6%	
	2	2-1	2.440		11.6%	
		2-2	2.439		12.0%	
	3	3-1	2.439		11.6%	
		3-2	2.404		12.3%	
	4	4-1	2.440		11.8%	
		4-2	2.444		11.6%	
	5	5-1	2.419		12.4%	
		5-2	2.417		12.2%	

173

3.2. Isothermal drying test

Figure 2 presents the variations of the specimens' mass loss versus time all along the drying experiment. The experimental mass loss $\left(\frac{\Delta m}{m}\right)$ was calculated for each specimen as follows:

$$\left(\frac{\Delta m}{m}\right)(t) = \frac{m(0) - m(t)}{m(0)} \tag{7}$$

where $m(0)$ and $m(t)$ are the initial mass of the specimen and the mass at time t respectively.

It is interesting to note that the fieldcrete behaved differently compared to the labcrete: the mass loss was always significantly greater (in line with the porosity that was higher) as well as the discrepancy. Here again, the five different batches as well as the difficulty of the concreting operations onsite may be held responsible.
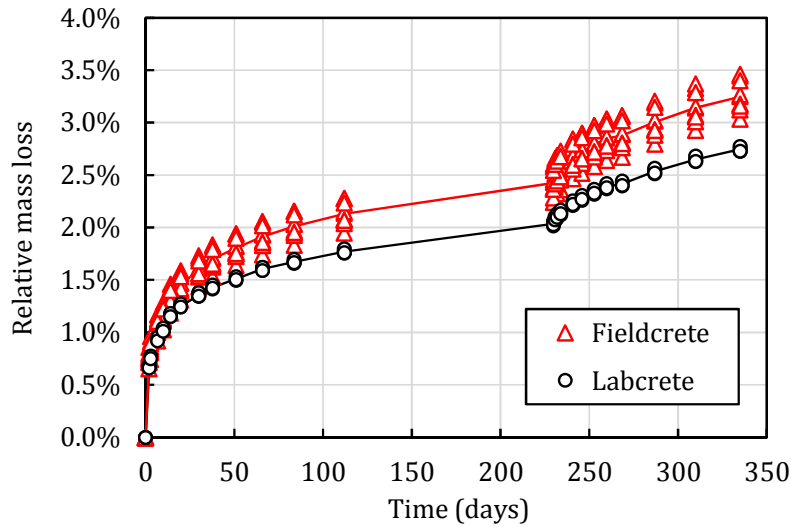
Figure 2 – mass loss variation versus time

3.3. Permeability assessment

In a first step, the intrinsic permeability was evaluated using inverse analysis independently on the two RH steps (55% and then 30%). The process detailed in section 2.3 was applied to all the specimens. Following Mualem's suggestion [47] and without relevant information about its value, the pore-interaction factor α was taken equal to +0.5 (1st run, Table 3). Separate simulations were conducted for each specimen considering individual data, namely density, porosity and mass loss (Table 2). The permeability assessment was done in two consecutive steps. Firstly, the process detailed in section 2.3 was used to assess the permeability of all the specimens using the results of the first drying phase only (55% RH). In a second step, the results of the second drying phase (30% RH) were used in the same way to assess the permeability of all the specimens once again. In that case, the permeability was assumed to be a piecewise function of time (cf. Figure 3): during the first 230 days (first drying phase at 55% RH) the permeability was fixed to the value obtained in the first simulation and after that the permeability value was adjusted to reproduce the experimental mass variations during the second drying phase (30% RH).
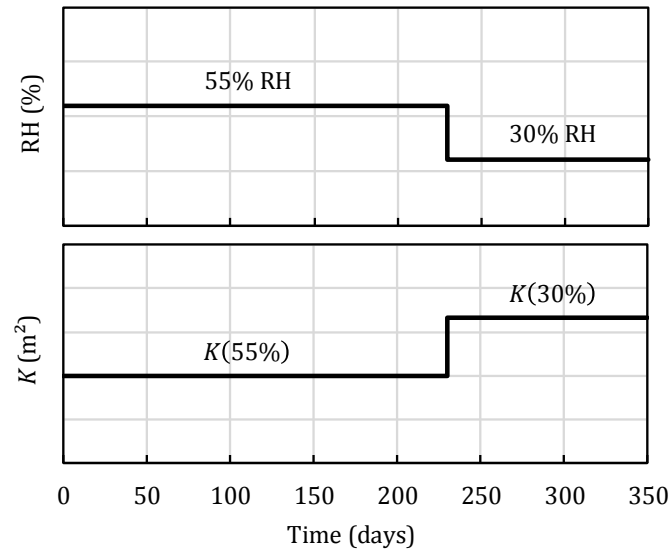
Figure 3 – RH and permeability for the 1st run of drying simulations

This approach yielded two different intrinsic permeability values for each specimen: $K(55\%)$ and $K(30\%)$ that are presented on Figure 4. The variability obtained for the fieldcrete was always significantly greater than that of the labcrete (about 4 times) in accordance with the experimental mass loss results (Figure 2).

Table 3 - summary of the simulations

| Parameters/properties		1st run	2nd run
Porosity	$\emptyset$	See the individual values of	See the individual values of
Density	d_s	Table 2	Table 2
van Genuchten exponent	m	0.532	0.532
van Genuchten pressure	P_0	59.05 MPa	59.05 MPa
Pore interaction factor	α	+0.5	α and K adjusted together
Intrinsic permeability	K	adjusted on the two RH steps (30% & 55%) resulting in two distinct values	using the results of the two RH steps (30% & 55%) resulting in a unique dataset

It is noteworthy that the intrinsic permeability values obtained at 30% RH were higher than those of 55% RH (by a factor 2-3, see 1st run in Table 4). This indicated that the relative permeability k_r was not correctly estimated and more specifically the slope between 55% and 30% RH was overestimated. This was due to the choice of the α value (+0.5) that did not

212 properly describe the relative permeability variations of the considered concrete. This is known

213 to induce significant discrepancy in the assessment of the intrinsic permeability over different

214 RH ranges [41].
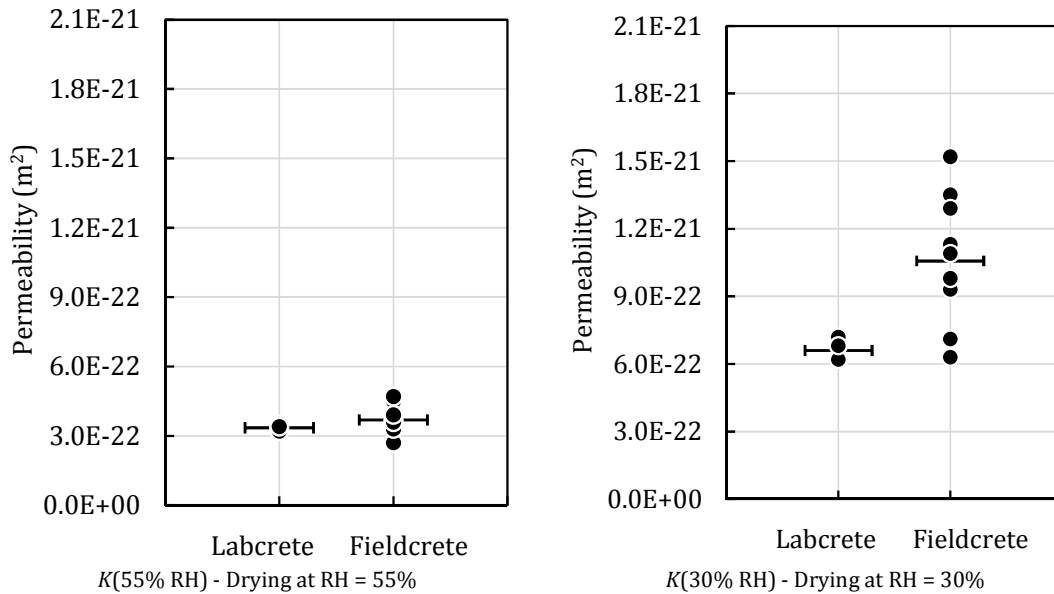
215 *Figure 4 – intrinsic permeability assessment using $\alpha = +0.5$*

216 In a second step, the pore interaction factor α was considered as an unknown empirical

217 parameter that needed to be calibrated together with the intrinsic permeability K as it is

218 commonly done in soil science [48–53] (2nd run, Table 3). The value of α was adjusted so that the

219 effective permeability (*i.e.* the product $K \times k_r$) matched the two different effective

220 permeabilities assessed at 55% and 30% RH (see the two black spots on Figure 5). The α-values

221 thus obtained are reported in Table 4 (column '2nd run'). In so doing, it was believed that the

222 slope of the effective permeability curve was correctly calibrated (at least between 55% and

223 30% RH).
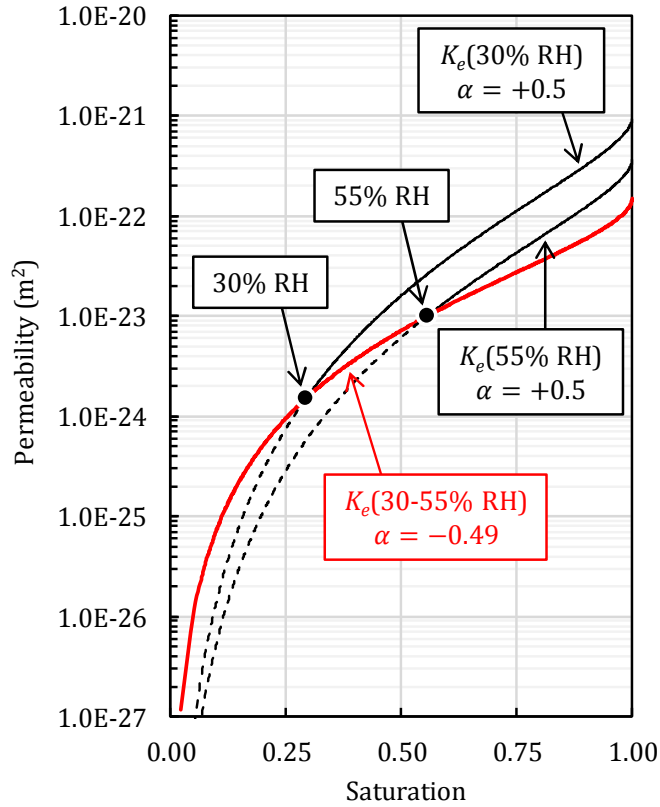
225 *Figure 5 – calibration of the pore-interaction factor α (example of the fieldcrete specimen 1-1)*

226 New simulations of the drying experiments were conducted for all the concrete specimens using

227 the pore interaction factor values that were obtained above. For each specimen a unique value of

228 intrinsic permeability was identified that made it possible to describe the mass loss variation all
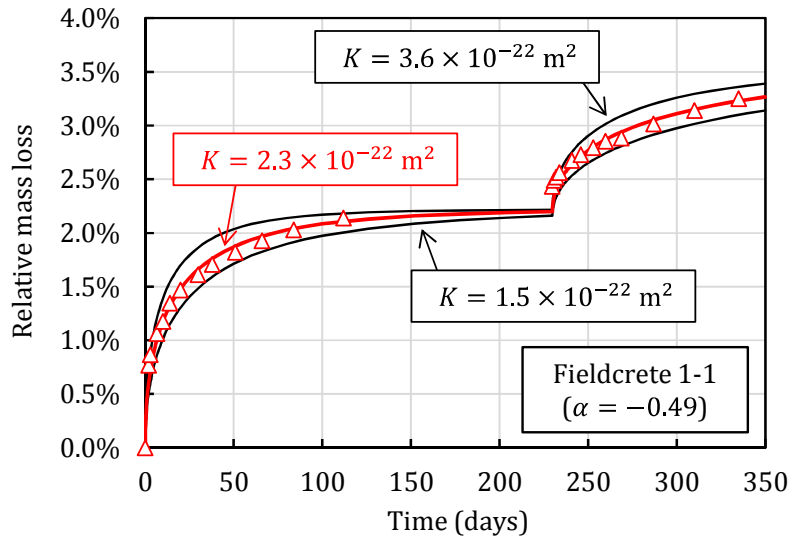
229 along the drying experiment (see 2nd run in Figure 6). This proved that the pore interaction

230 factor α was properly evaluated and that the resulting data set could be used to describe

231 accurately the water exchange with the environment down to 30% RH.

4.0%

3.5%

3.0%

2.5%

2.0%

1.5%

1.0%

0.5%

0.0%

Relative mass loss

$K = 3.6 \times 10^{-22} \text{ m}^2$

$K = 2.3 \times 10^{-22} \text{ m}^2$

$K = 1.5 \times 10^{-22} \text{ m}^2$

Fieldcrete 1-1
$(\alpha = -0.49)$

0   50   100   150   200   250   300   350

Time (days)

Figure 6 – new assessment of the intrinsic permeability K using α ≠ +0.5 (example of the fieldcrete specimen

1-1)

All the results in terms of permeability and pore interaction factor are reported in Table 4 and

plotted in Figure 7. It is interesting to note that after the second assessment step, the intrinsic

permeability values obtained for the fieldcrete were very close to those of the labcrete (Figure

8). This was not the case after the first step. Reevaluating the pore interaction then helped to

improve the accuracy of the evaluation and eventually show that the labcrete and fieldcrete

were very similar in terms of intrinsic permeability (2×10^{-22} m²). The reader must keep in mind

though that the intrinsic permeability assessed using inverse analysis depends on the model and

input data used [42]. One can wonder whether the conclusion would have been the same using a

different evaluation process.

All the pore interaction factors presented negative values that were different for the labcrete

and fieldcrete: they ranged between -0.5 to -0.6 for the labcrete and between -1.0 to -1.4 for the

fieldcrete. It is noteworthy that all these values were different from the value suggested by

Mualem (+0.5). This has been known for long for soils for which many results were published

[47–50,53–55]. In the field of cement-based materials, results are scarce. A positive value of +5.5

was proposed using gas permeability tests [2,56] but negative values were obtained by Leech et

al. [57] using capillary absorption tests: they obtained values ranging from -0.2 to -1.2. Later

251 Poyet *et al.* [41] dried partially carbonated specimens with decreasing RH steps and after

252 inverse analysis obtained values ranging from -1.5 to -4.0. It is interesting to note that the values

253 obtained in this study for the labcrete matched the proposition of Leech *et al.* to use $\alpha = -0.5$

254 instead of +0.5 [57]. The α-values of the fieldcrete were somewhat lower (-1.2 in average).

255 In terms of experimental scatter, the variability of the intrinsic permeability of the labcrete was

256 very low: the coefficient of variation was 3%. This was expected because all the four specimens

257 were carefully fabricated in the laboratory using the same concrete batch. The coefficient of

258 variation of the fieldcrete was found to be higher (12%) because the specimens originated from

259 five different concrete batches that were fabricated onsite by the workers in charge of the

260 realization of the surface disposal mockup. The coefficient of variation that was found for the

261 fieldcrete however remained limited compared to the values obtained in other studies – see for

262 instance [44] - indicating that it is possible to limit the variability of concretes *in situ*.

263

264 *Table 4 – intrinsic permeability and pore interaction factor data*

Concrete	Batch	Specimen	1st run			2nd run	
			α	K(55% RH)	K(30% RH)	α	K
Labcrete	1	I	+0.5	3.3×10^{-22}	6.2×10^{-22}	-0.49	2.2×10^{-22}
		II	+0.5	3.2×10^{-22}	6.2×10^{-22}	-0.54	2.1×10^{-22}
		III	+0.5	3.5×10^{-22}	7.2×10^{-22}	-0.63	2.2×10^{-22}
		IV	+0.5	3.4×10^{-22}	6.8×10^{-22}	-0.59	2.2×10^{-22}
Fieldcrete	1	1-1	+0.5	3.6×10^{-22}	9.4×10^{-22}	-1.00	2.3×10^{-22}
		1-2	+0.5	2.7×10^{-22}	7.1×10^{-22}	-1.02	1.7×10^{-22}
	2	2-1	+0.5	3.5×10^{-22}	11.0×10^{-22}	-1.30	1.6×10^{-22}
		2-2	+0.5	3.7×10^{-22}	11.3×10^{-22}	-1.25	2.2×10^{-22}
	3	3-1	+0.5	3.4×10^{-22}	9.3×10^{-22}	-1.08	2.1×10^{-22}
		3-2	+0.5	4.5×10^{-22}	15.2×10^{-22}	-1.41	2.6×10^{-22}
	4	4-1	+0.5	3.3×10^{-22}	9.8×10^{-22}	-1.21	1.9×10^{-22}
		4-2	+0.5	3.6×10^{-22}	10.9×10^{-22}	-1.24	2.1×10^{-22}
	5	5-1	+0.5	4.7×10^{-22}	13.5×10^{-22}	-1.15	2.7×10^{-22}
		5-2	+0.5	3.9×10^{-22}	12.9×10^{-22}	-1.38	2.2×10^{-22}

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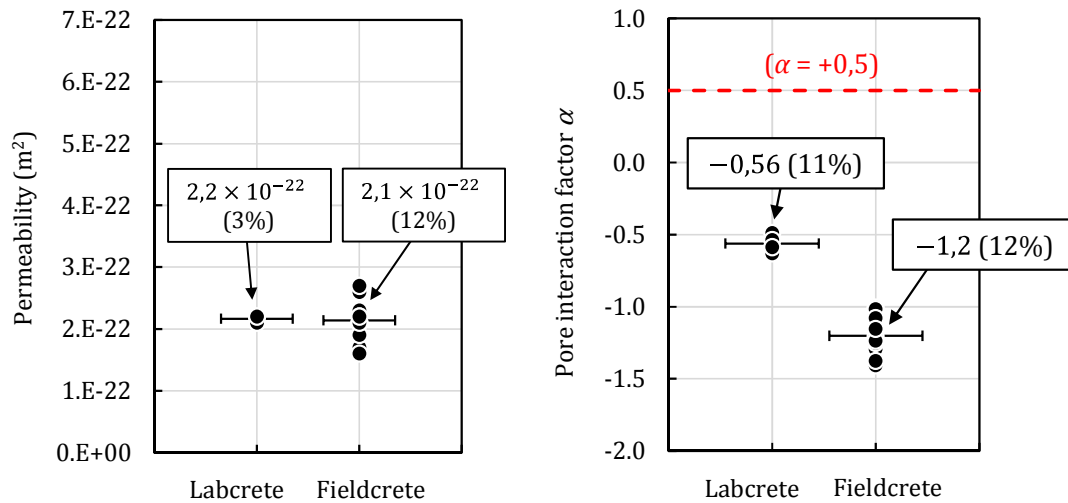
Figure 7 – intrinsic permeability K (left) and pore interaction factor α (right) of the concrete specimens

Figure 8(a) compares the unsaturated permeability evolutions for all the tested specimens. Although the intrinsic permeability values (S=1) were more or less the same for the labcrete and the fieldcrete, the fieldcrete specimens were always more permeable than the labcrete ones. At 55% RH (S=0.555), the effective permeability of the fieldcrete was between once and twice that of the labcrete. At 30% RH (S=0.293), the effective permeability of the fieldcrete was between 1.4 and 3.4 times that of the labcrete (Figure 8(b)). This was due to the differences in pore-interaction factor α (Figure 7) that influenced the slope of the effective permeability. It is noticeable that, below 30% RH, the fieldcrete permeability steeply increased faster than that of the labcrete when saturation decreased. The fieldcrete permeability could then be ten times higher than that of the labcrete for very low saturation values. However this point was not judged significant for two reasons. Firstly, it must be recalled that this increase was obtained for RH values that were much lower than 30%; these values are almost never encountered in real life. Secondly, the increase was obtained for saturation values that were very far from the RH-domain in which the permeability was evaluated. This increase might then be somewhat questionable.
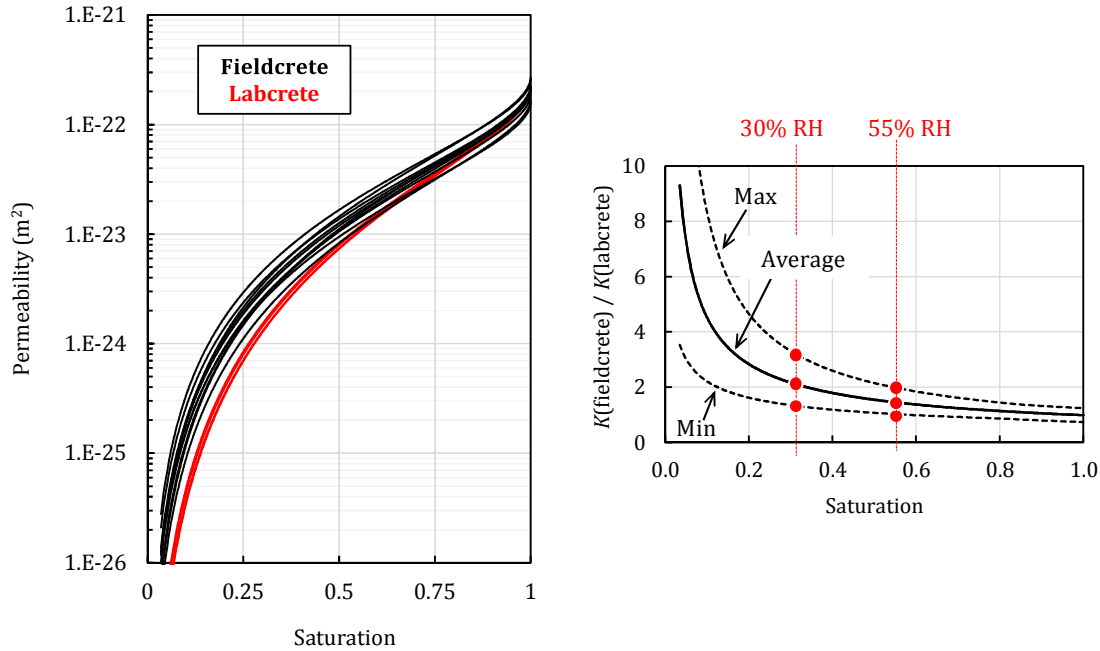
(a) unsaturated permeability evolution of all the tested specimens

(b) ratio of the fieldcrete permeability to that of the labcrete

Figure 8 – unsaturated permeability evolutions for all the labcrete (in red) and fieldcrete (in black) specimens

4. Application: simulations of drying

4.1. 1D simulation of a homogeneous material

To illustrate the effects of the identification procedure on the saturation degree profiles, we propose to simulate in this section the case of a homogeneous material subjected to drying at constant relative humidity. The parameters identified in the previous section will be successively adopted and the obtained results will be compared. The structure considered consists of a fraction of concrete wall with thickness 20 cm, and with its two opposite faces exposed to a relative humidity of 55% (see Figure 9). The drying phenomenon is assumed to occur perpendicularly to these faces and is one-dimensional, though the resolution of the problem is 2D. For symmetry reason, only half of the structure is considered. Again, the finite element code Cast3m is used to solve eq. (1), with 400 elements having variable dimensions (their size is smaller near the exposed surface to capture accurately the high gradients appearing when the loading is applied, and increases progressively) to discretize the structure.

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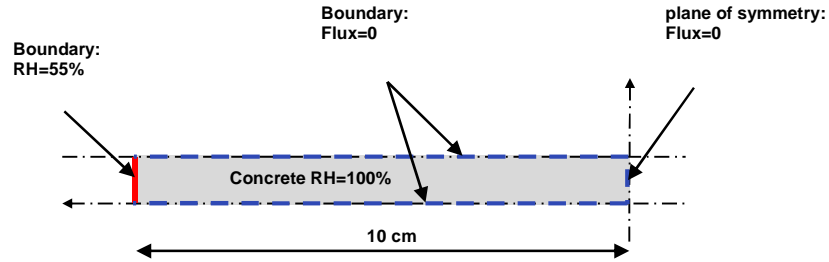
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299
Figure 9 – schematic description of the 1D simulations and boundary conditions

300   The first simulation is intended to compare the results of labcrete and fieldcrete corresponding

301   to the identification procedure with $\alpha \neq 0.5$ shown in Figure 7, *i.e.* for the mean values of

302   parameters for both materials. Note that the respective average value of porosity (see Table 2) is

303   used for each case. The saturation degree profiles obtained at 100 days, 1 year and 3 years of

304   drying are plotted in Figure 10 as a function of the depth, x=0 designating the exposed face. Very

305   few differences can be observed between labcrete and fieldcrete profiles, indicating that on

306   average the two materials exhibit similar drying processes and then close permeability

307   properties in unsaturated conditions.
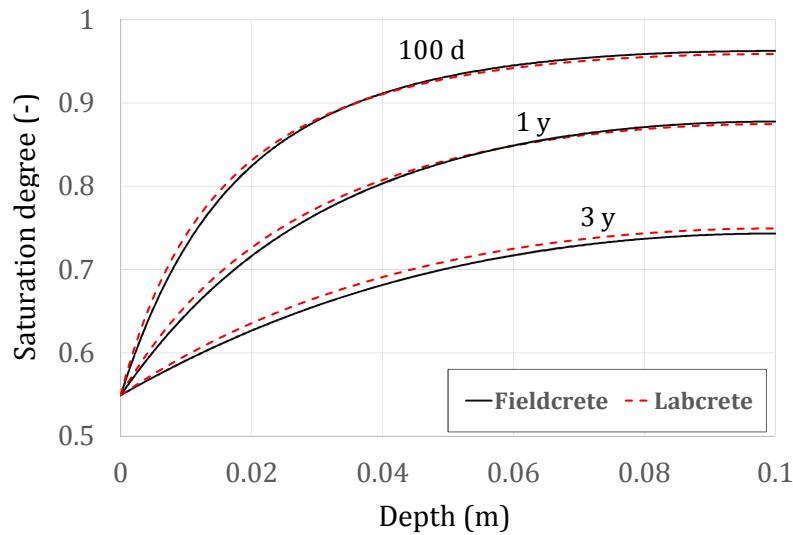
308

309

310   *Figure 10 – saturation profiles at 100 days, 1 year and 3 years for labcrete and fieldcrete obtained with the*

311   *parameters of Figure 7*

312   We now examine the influence of the permeability value retained for the identification (i.e., at 30

313   and 55% HR, see Figure 5 and Table 4, 1st run) on the description of the drying kinetics when the

314   parameter α is kept equal to 0.5. Figure 11 presents the saturation profiles obtained at 100 days

315   and 3 years in the case of fieldcrete 1.2 and 3.2, and for the two values $K(55\%)$ and $K(30\%)$.

316   These cases are chosen because they appear to envelop all curves with the $\alpha = -1.2$

317   identification procedure (see Figure 12). For the sake of comparison, we also reported in dotted

318   lines the curves simulated with $\alpha = -1.2$ and shown on Figure 10.
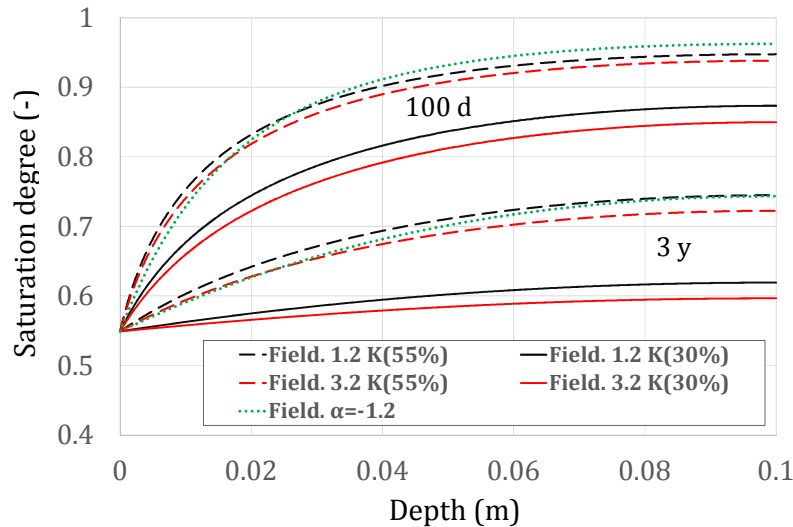

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320

321   *Figure 11 – saturation profiles at 100 days and 3 years for fieldcrete 1.2 and 3.2 obtained with parameters*

322   *$\alpha = 0.5$ and two values of permeability; comparison with the identification of Figure 7 ($\alpha = -1.2$)*

323   We first observe that the saturation profiles simulated with the two permeability values exhibit

324   very significant differences. Further, the $K(55\%)$ curves are at the same time close to each other

325   and close to the $\alpha = -1.2$ average case. This is not very surprising since the validity domain of

326   the parameters identified at 55% is more consistent with the practical RH domain covered in the

327   simulation than the one identified at 30%. Finally, we conclude that the $K(55\%)$ with $\alpha = 0.5$

328   values provide saturation profiles in good concordance with those obtained with the $\alpha = -1.2$

329   identification method.

330   Figure 12 presents the saturation profiles obtained at 100 days, 1 year and 3 years for all

331   labcrete (top) and fieldcrete (bottom) specimens calculated with the parameters of the 2nd run of

332   Table 4 corresponding to $\alpha \neq 0.5$. We observe that for labcrete, the curves are relatively close

333   whatever the samples considered, while for fieldcrete the scatter is as expected much more

334   significant. Although we may argue that the greater number of fieldcrete specimens also

335   contributes to this larger variability, the more disperse response for these concrete samples

336   appears clearly and leads to important differences in saturation profiles.
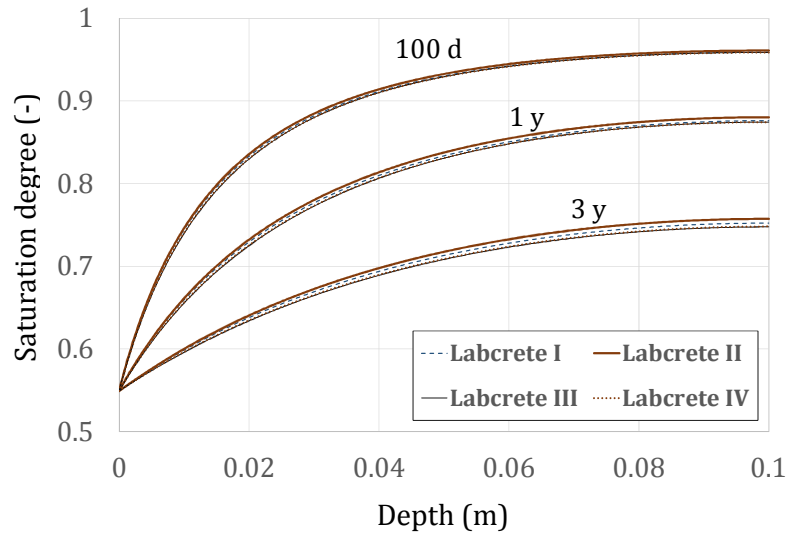
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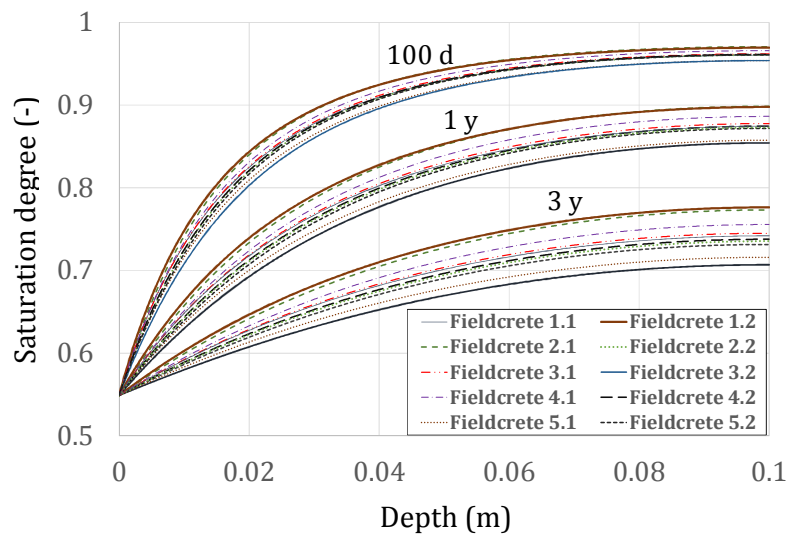
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340

341   *Figure 12 – saturation profiles at 100 days, 1 year and 3 years for all labcrete (top) and fieldcrete (bottom)*

342   *specimens calculated with the parameters of the 2ⁿᵈ run of Table 4*

343

344   These results are totally in line with those shown on Figure 2 and Figure 8. The discrepancies in

345   the saturation degree profiles increase as a function of time (at least up to 3 years), which means

346   that the time needed for obtaining a quasi-homogeneous saturation profile may differ

347 considerably in particular between the fieldcrete specimens. As a corollary, the question of the

348 notion of representative elementary volume is posed as it may not to be the same for labcrete

349 and fieldcrete, *i.e.* a greater volume is expected for fieldcrete to appropriately represent the

350 material with a variability similar to the labcrete one.

351 Among the possible causes of the greater variability in the fieldcrete results, a more significant

352 dispersion in the spatial repartition of the different components (aggregates, cement paste,

353 pores) due to a lower homogeneity in the casting procedure, and the variability in the actual

354 formulation, are expected to be of importance. We propose to examine the first aspect in the

355 next section through simulations of mesoscale concrete specimens exhibiting a different
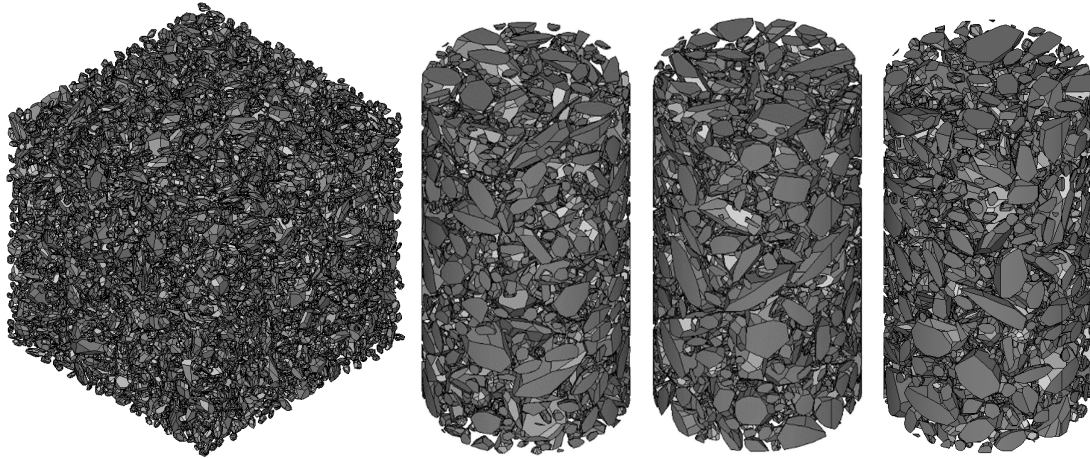
356 aggregate distribution.

357

4.2. Simulation of 3D concrete samples

359 To investigate the role of the aggregates within the specimens on the overall drying kinetics, we

360 propose to perform mesoscale 3D simulations on numerical samples generated with different

361 aggregate distributions and shapes. Such mesoscale simulations on concrete representative

362 volumes involving explicitly the aggregates are increasingly used due to the growing power of

363 computers to analyze various effects and characterize properties related to (possibly coupled)

364 mechanical, diffusive and chemical problems, see for instance [58–61] In this paper, to be as

365 close as possible to the experimental conditions of fieldcrete testing, the numerical samples are

366 constructed following the experimental procedure, *i.e.* cubic concrete volumes with dimensions

367 15×15×15 cm are generated, from which cylindrical samples of diameter 6 cm and height 11 cm

368 are extracted (cored). The aggregate dimensions are imposed by the actual grading curve. Note

369 that the aggregates are generated numerically with convex polyhedral shapes obtained by a

370 Voronoi space decomposition, which is a notable difference with *e.g.* [61] in which aggregates

371 are spherical. The aggregates are next modified to conform to a prescribed aspect ratio

372 randomly chosen between 1 and 4 along two perpendicular directions, so as to generate

373   flattened/elongated shapes. The numerical procedure makes use of the functionalities of the

374   CAD code Salome (www.salome-platform.org), and is described in more details in *e.g.* [62–64].

375   Although these numerical aggregates are expected to be relatively realistic, the obtained

376   approximated shapes (in particular, real aggregates are not in general convex) may introduce a

377   certain bias in the results. However it has been reported in [65] that regarding viscoplastic

378   mechanical behavior, such numerical aggregates reproduce relatively well the overall concrete

379   behavior when compared to real aggregates obtained by tomography. A similar study regarding

380   transport properties would be necessary to investigate the impact of real versus numerical

381   aggregates.

382   Figure 13 left presents a generated cubic specimen with 12370 aggregates (left), corresponding

383   to an aggregate volume fraction of 35% and a minimum size on the grading curve of 3.6 mm.

384   Such ratio is deemed to be sufficiently realistic to achieve representative results, while keeping

385   the computation costs reasonable. Note that the random process of particle placing accounts for

386   a minimum distance between aggregates, and has to fulfill the non-overlapping condition with

387   the cube surfaces. Figure 13 right shows the aggregate distribution in 3 cylindrical specimens

388   cored from different cubic samples. For the simulations, 6 samples have been extracted from 3

389   different cubes. Interestingly, the aggregate volume fraction calculated in the specimens ranges

390   between 0.374 and 0.383, which is significantly higher than the one imposed in the initial cubic

391   volumes due to the wall-effect and corresponding non-homogeneity of the aggregates

392   repartition in the cubes between regions near the surfaces and the core.

393

394   *Figure 13 – example of 15×15×15 cubic specimen generated with 12370 aggregates (left); aggregate*

395   *distribution in 3 cylindrical specimens constructed from the cubic samples (right)*

396   The meshes are generated automatically by the meshing softwares MG-CADSurf and MG-Tetra

397   developed by Distene[4], and plugged in Salome. The total number of tetrahedral elements in the

398   meshes of the cylindrical specimens range between 2.26 and 2.32×10^6. The simulations consist

399   of a drying test from an initial totally saturated state during 1 year, and with the lateral surfaces

400   of the specimens exposed to an environment with RH = 0.55. To focus on the aggregate shape

401   effects and ease the comparison, the material parameters of the matrix phase (corresponding

402   here to the mortar) are supposed to be the same for all samples, and are taken as $K = 2 \times 10^{-22}$ m²,

403   $\alpha = -0.56$, and $\phi = 0.2$. Note that as the values of K and α are not identified experimentally on

404   mortars, they are simply set from those determined for concretes in the previous sections, given

405   that we do not expect that the results regarding the effects of aggregate shapes would be

406   different with (slightly) altered values. The macroscopic transport properties obtained on the

407   numerical specimens with these values for mortar are calculated and discussed in the sequel.

408   The aggregates are not accounted for in the calculations since they are supposed to be non-

409   diffusive. Also, the possible preferential pathways for transport at the interfaces between

410   aggregates and matrix (the so-called ITZ) are ignored here. Indeed, we assume that, as by

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[4] http://www.distene.com

411 construction these interfaces do not form a connected network, their impact on the overall

412 results is weak.

413 Figure 14 presents the simulation results in terms of time evolution of overall saturation degree

414 (left) and water mass (right) calculated within all 6 specimens. The mass of water is simply

415 obtained from the saturation degree and the average porosity in the whole samples, *i.e.* the

416 porosity corrected by the volume fraction of matrix. We can observe that the saturation degree

417 curves are identical for all cases, while the water mass ones exhibit a slight difference. The latter

418 are mainly attributed to the different mean porosity in the samples, which is a consequence of

419 the variable volume fraction of matrix due to the random generation process of the numerical

420 samples. From these results, we may assert that, on average, the global drying response is nearly

421 the same for the specimens. This indicates that regarding the saturation degree averaged over

422 the entire volume, the influence of the aggregate distribution as investigated in this section is

423 negligible.

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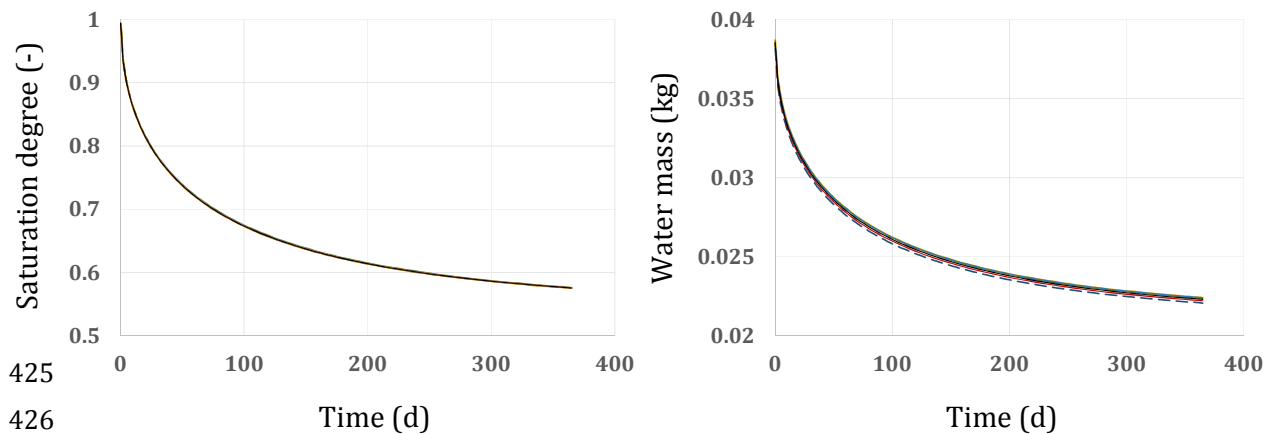
427 *Figure 14 – evolution of the overall saturation degree (left) and mass of water (right) for the 6 calculated*

428 *specimens*

429 As mentioned above, it may be instructive to characterize the macroscopic (or equivalent)

430 transport parameters of the generated numerical concretes, from the results of water mass loss

431 of Figure 14 as done in section 3 from experiments, and to compare them with the input data of

432 mortar. Assuming the same value of α for both materials, *i.e.* $\alpha = -0.56$, we then propose to

433 apply the inverse analysis procedure described above to identify the permeability coefficient.

434 Figure 15 presents the curves obtained on a homogeneous cylinder of diameter 6 cm and height

435 11 cm with different values of K (continuous lines), and the mean curve resulting from the 3D

436 numerical simulations on the 6 reconstructed specimens (points). The comparison indicates that

437 the value K=0.75×10^{-22} m² leads to a water mass loss kinetics very close to the numerical

438 concrete one. This means that the hypothesis on the value of $\alpha = -0.56$ is relevant for the

439 homogenous material; on the other hand, the permeability coefficient K is significantly lower

440 than the one of the mortar.
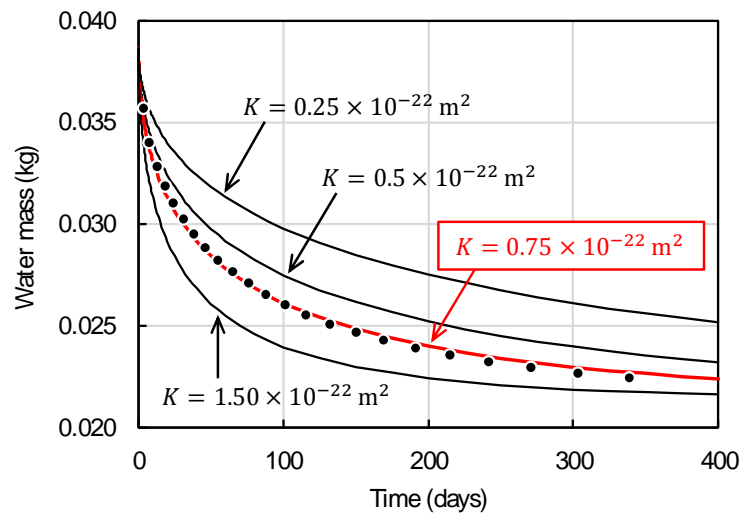
441

442 *Figure 15 – evaluation of the average permeability of the 6 reconstructed 3D specimens using inverse*
443 *analysis (they were considered as homogeneous materials)*

444

445 It is important to notice that while the identification procedure is performed on a material

446 assumed as homogeneous, hence with its entire boundary surfaces exposed to drying, the

447 exchange of water takes place only through the contact surfaces between mortar and

448 atmosphere in the 3D simulations, since the aggregates that overlap the lateral surfaces are non-

449 diffusive. This means that the surface exposed to drying is much lower in the latter case than in

450 the former one, which may according to the authors explain at least partly the important

451 difference between macroscopically identified permeability coefficient and the prescribed input

462 To investigate in more details the numerical results on the 3D specimens, Figure 16 shows the

463 saturation degree profiles in the 6 samples at 5 days, 100 days and 1 year. The horizontal axis

464 designates the radius of the specimens, with 0 being the center and 0.03 the external surface.

465 The curves are obtained by averaging the calculated saturation degree fields on cylindrical

466 surfaces whose axis is identical to the samples one and whose radius evolves progressively from

467 0 to 0.03. Compared to Figure 14 showing volume-averaged quantities, Figure 16 then presents

468 surface-averaged results, which are deemed to provide more insightful and accurate information

469 about the aggregate distribution effects. We observe however that the curves for the different

470 specimens cannot be really distinguished; only a very small discrepancy may be seen on the 100

471 days results. This means that, in line with the conclusion on Figure 14, the saturation degree

472 profiles are not significantly affected by the aggregate distribution as considered here.

473 Finally, Figure 17 presents the numerical results in a more local manner than the two previous

474 Figures, with the saturation degree averaged over circles centered on the specimen axis. The

475 procedure is basically similar to the one leading to Figure 16, except that the cylindrical surfaces

476 of interest are here sampled by plans perpendicular to the axis. The idea is to examine the

477 evolution of the saturation degree along the axial direction at prescribed distances from the

478 surface exposed to drying, and at different times. We propose to analyze the results near the

479 lateral surface at the radius $r = 0.027$ m, and also at mid-distance between the axis and the

480 surface at the radius $r = 0.015$ m, corresponding to Figure 17 top and bottom, respectively, and

481 at 5, 25 and 100 days. The abscissa designates the position of the points along the axis, with 0

482 being arbitrarily the lower cross-section of the specimens. We observe that the results at

483 $r = 0.027$ (top) exhibit non-negligible variations along the axis direction, but also between the

484 different specimens. This is particularly visible at the onset of drying (5 days), while the curves

485 tend progressively to homogenize at greater times, with differences becoming relatively weak at

486 100 days. Maximum discrepancies of about 4.5% and 2.5% are reported at 5 days and 100 days,

487 respectively. The results at $r = 0.015$ show an opposite tendency: from the initial prescribed

488 homogeneous state, the saturation degree turns out to gradually disperse for increasing times,

489 though moderately; at 100 days, the maximum difference between all results is less than 3%.

490 To sum up, the curves of Figure 17 indicate that the aggregates influence locally the drying

491 phenomenon all the more that the gradients of saturation degree (or equivalently of capillary

492 pressure) are high, *i.e.* the kinetics of transport is rapid. At the beginning of the simulations these

493 gradient are maximal near the exposed surfaces, and the presence of aggregates as obstacles to

494 water transfer is noticeable. By contrast, when gradients are low as in the specimen centers or at

495 greater times, their influence and correspondingly their size and shape distribution, become

496 more and more negligible.
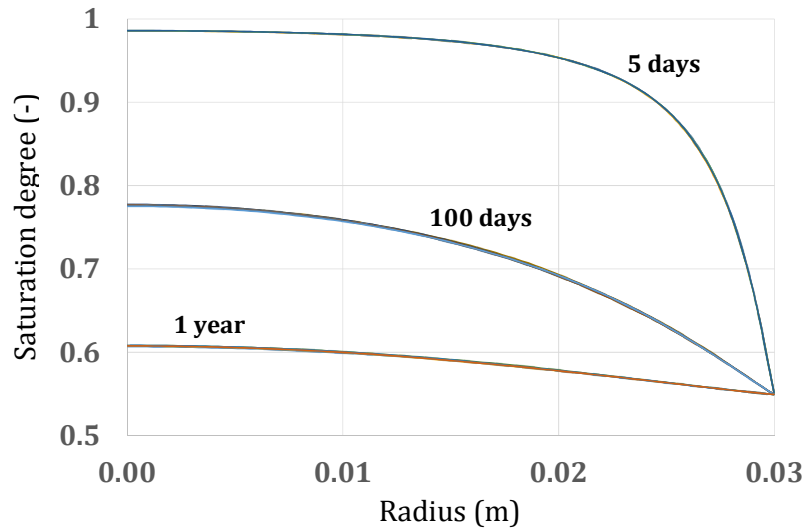
Figure 16 – saturation degree profiles as a function of the radius for the 6 calculated specimens at 3 different times

To conclude with the 3D numerical simulations presented in this subsection, the spatial distribution of aggregates within the samples seem to have a limited impact on the drying characteristics. When examining saturation degree evolutions as volume- and surface- averaged quantities, this aspect is clearly negligible. Locally, the influence of aggregates is visible in the zones where the gradients of capillary pressures are high, *i.e.* essentially at the beginning of drying near the exposed surfaces. Note that in practice, due to cyclic and seasonal environmental conditions, significant gradients may persist in these zones, meaning that the involved aggregates may have a certain impact on the kinetics.

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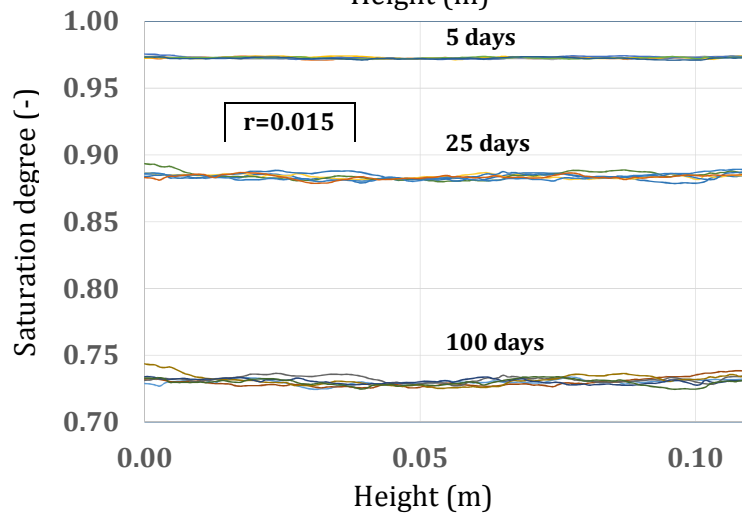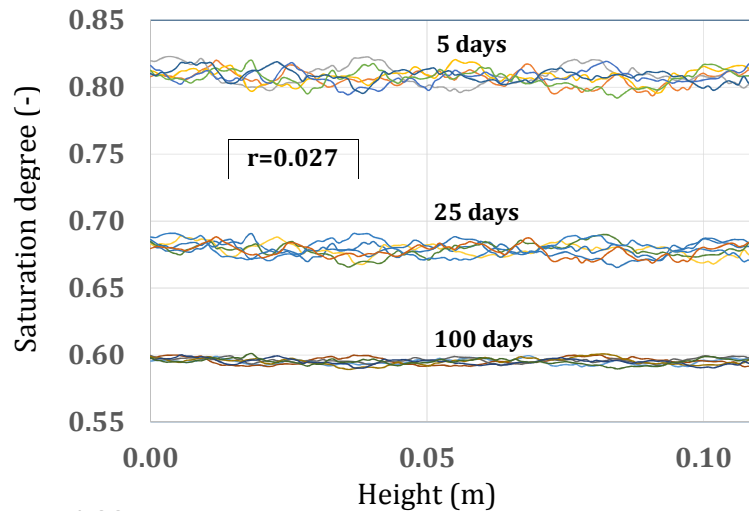512   *Figure 17 – saturation degree profiles as a function of the radius for the 6 calculated specimens at 3 different*

513   *times.*

514   Overall, considering all the other factors as constant, the variability in the (coarse) aggregate

515   distribution as investigated here cannot explain the dispersion observed experimentally in the

516   fieldcrete (and also to a lesser extent in the labcrete) specimens. Some other reasons should be

517   pointed out, as the variability in the formulation and in the phase properties of the cement paste.

518   To be addressed, these aspects would need to be characterized experimentally, which

519   constitutes a challenging aspect.

520

5. Conclusion

In order to characterize the difference in permeability between labcrete and fieldcrete, the unsaturated permeability to water of a modern concrete was evaluated using inverse analysis. Labcrete specimens were prepared and cured in the laboratory and fieldcrete specimens were prepared during the construction of test panels (ca 25m^3). The fieldcrete appeared to be more porous than the labcrete (11.9% in average vs. 10.6%) but, using inverse analysis and accounting for water permeation only, the intrinsic permeability values were very close for the two concretes (2.2×10^{-22} and 2.1×10^{-22} in average for the labcrete and fieldcrete, respectively). The fieldcrete however exhibited lower pore-interaction factor (*i.e.* the parameter of Mualem's model that accounts for pore structure tortuosity and connectivity) than the labcrete (-1.2 vs. -0.56), indicating that the tortuosity and connectivity of the poral network were not the same for the two concretes. The fieldcrete also displayed more scatter, which can be mainly attributed to the five distinct batches that were considered. Clearly enough, non-negligible discrepancies were reported in the identified relative permeabilities for the two concretes, in particular for saturation degrees below about 0.7. These differences increased for decreasing values of saturation, the relative permeability of fieldcrete remaining higher. This means that the drying kinetics of fieldcrete would be potentially faster for low saturation, but in practical environmental conditions such small saturation states are likely to be rarely met.

Moreover, one-dimensional simulations performed on a saturated homogeneous concrete wall subjected to drying at HR=55% showed very little differences between fieldcrete and labcrete (with model parameters prescribed as the averaged ones) in terms of saturation degree profiles at various times. By contrast, important variations were observed when the parameters identified on the various fieldcrete specimens were successively considered in the calculations. Finally, as a first attempt to investigate the effects of the aggregate distribution on the variability observed on the experimental results, 3D mesoscale simulations were carried out on reconstructed cylindrical specimens of same dimensions as the tested ones. Only the aggregate

547 distributions and shapes were varied between the 3 generated cubes where the 6 samples were

548 cored. This resulted in slight variations of aggregate volume fraction between the specimens.

549 Overall, the main results indicated that the evolutions of volume-averaged saturation degrees

550 and surface-averaged saturation degree profiles were almost identical for all 6 specimens. Only

551 by examining the saturation degree at given distances from the exposed surface along the axis

552 direction of the samples can be observed non-negligible variations, in particular near the surface

553 where the saturation gradients are higher. This means that the different aggregate distributions

554 between numerical specimens lead to significant local saturation disparities, but cannot alone

555 explain the observed macroscopic variability. An important part may originate from the matrix

556 properties themselves (*i.e.* spatial variability in the content, the porosity, the placement etc.),

557 which are however quite difficult to characterize experimentally. This aspect would deserve to

558 be addressed, both on the numerical and experimental grounds.

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